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C:\atnweb\Queries\838.str
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```
ring bonds:

1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 8-9

exact/norm bonds:

1-2 1-5 4-5 4-6 5-9 6-7 7-8 8-9

exact bonds:

2-3 2-11 3-4 3-10

isolated ring systems:

containing 1:

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
```

chain nodes : 10 11

2-11 3-10

ring nodes:
1 2 3 4 5 6 7 8 9
chain bonds:

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FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 21 JUL 2003 HIGHEST RN 552272-14-7 DICTIONARY FILE UPDATES: 21 JUL 2003 HIGHEST RN 552272-14-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

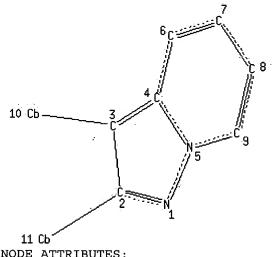
Experimental and calculated property data are now available. See HELF PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 , STR



NODE P	TTRI	3 O.1	res:		
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NSPEC	IS	R		AT	2
NSPEC	IS	R		AΤ	3
NSPEC	IS	R		ΑT	4
NSPEC	IS	R		ΑT	5
NSPEC	IS	R		AT	6
NSPEC	IS	R		AΤ	7
NSPEC	IS	R		AT	8
NSPEC	TS	R		AΤ	9

NSPEC IS C AT 10
NSPEC IS C AT 11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

=> s 11

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SAMPLE SCREEN SEARCH COMPLETED - 1901 TO ITERATE

52.6% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

8 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

35405 TO 40635

PROJECTED ANSWERS:

71 TO 537

L2 8 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 13:53:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 38061 TO ITERATE

100.0% PROCESSED 38061 ITERATIONS SEARCH TIME: 00.00.01

186 ANSWERS

DEARCH TIME. 00.00.01

L3 186 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 152.55 152.76

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FILE COVERS 1907 - 22 Jul 2003 VOL 139 ISS 4

FILE LAST UPDATED: 21 Jul 2003 (20030721/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

′ 9 L3 L4

=> s 14 and pd < december 1998 18904707 PD < DECEMBER 1998

(PD<19981200)

L5 3 L4 AND PD < DECEMBER 1998

=> s 14 and campbell, i?/au

1545 CAMPBELL, I?/AU

2 L4 AND CAMPBELL, I?/AU L6

=> d 16, ibib abs fhitstr, 1-2

ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2003 ACS on STN

Citing Full References Text

2000:628138 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 133:222726

TITLE: Preparation of pyrazolopyridines as selective

inhibitors of COX-2

INVENTOR(S): Campbell, Ian Baxter; Lambeth, Paul Francis; Naylor,

Alan; Pegg, Neil Anthony

PATENT ASSIGNEE(S): Glaxo Group Limited, UK SOURCE: PCT Int. Appl., 40 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE				
							
WO 2000052008	A1 20000908	WO 1999-EP10263	19991222				
W: AE, AL	AM, AT, AU, AZ,	BA, BB, BG, BR, BY, CA,	CH, CN, CR, CU,				
CZ, DE	DK, DM, EE, ES,	FI, GB, GD, GE, GH, GM,	HR, HU, ID, IL,				
IN, IS	JP, KE, KG, KP,	KR, KZ, LC, LK, LR, LS,	LT, LU, LV, MA,				
MD, MG	MK, MN, MW, MX,	NO, NZ, PL, PT, RO, RU,	SD, SE, SG, SI,				
SK, SL	TJ, TM, TR, TT,	TZ, UA, UG, US, UZ, VN,	YU, ZA, ZW, AM,				
, AZ, BY	KG, KZ, MD, RU,	TJ, TM					
RW: GH, GM	KE, LS, MW, SD,	SL, SZ, TZ, UG, ZW, AT,	BE, CH, CY, DE,				
DK, ES	FI, FR, GB, GR,	IE, IT, LU, MC, NL, PT,	SE, BF, BJ, CF,				
CG, CI	CM, GA, GN, GW,	ML, MR, NE, SN, TD, TG					
EP 1157025 A1 20011128 EP 1999-968808 19991222							
R: AT, BE	CH, DE, DK, ES,	FR, GB, GR, IT, LI, LU,	NL, SE, MC, PT,				
IE, SI	LT, LV, FI, RO						
JP 2002538157 T2 20021112 JP 2000-602234 19991222							
<u>US 6498166</u>	B1 20021224	US 2001-890925	20010830				
PRIORITY APPLN. INFO.: GB 1999-4506 A 19990227			19990227				
,		GB 1999-20904 A	19990903				
		WO 1999-EP10263 W	19991222				
OTHER SOURCE(S): MARPAT 133:222726							

GI

I

The title compds. [I; R0, R1 = H, halo, alkyl, etc.; R2 = halo, CN, AΒ CONR4R5, etc.; R3 = alkyl, NH2; R4, R5 = H, alkyl, (un)substituted Ph; NR4R5 = satd. 4-8 membered ring] which are potent and selective inhibitors of COX-2 and are of use in the treatment of the pain, fever, inflammation of a váriety of conditions and diseases, were prepd. and formulated. E.g., a multi-step synthesis of I [R0 = 4-F; R1 = H; R2 = 6-CN; R3 = NH2]which showed IC50 of 21 nM against COX-2 vs. IC50 of 20,950 nM against COX-1, was given.

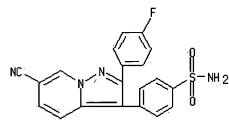
IT 291743-84-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrazolopyridines as selective inhibitors of COX-2)

RN291743-84-5 HCAPLUS

Benzenesulfonamide, 4-[6-cyano-2-(4-fluorophenyl)pyrazolo[1,5-a]pyridin-3-CN yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2003 ACS on STN L₆

2

Citing Full References Text

2000:314697 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 132:321858

Preparation of pyrazolopyridines as selective COX-2 TITLE:

inhibitors

INVENTOR(S): Campbell, Ian Baxter; Naylor, Alan

PATENT ASSIGNEE(S): Glaxo Group Limited, UK SOURCE: PCT Int. Appl., 46 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

English

Patent LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

KIND DATE APPLICATION NO. PATENT NO. DATE A1 20000511 WO 1999-EP8186 19991101 WO 2000026216

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,

IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG 20010807 BR 1999-15011 19991101 BR 9915011 Α 19991101 EP 1999-955897 EP 1127058 20010829 Α1 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, · IE, SI, LT, LV, FI, RO 19991101 JP 2002528547 T220020903 JP 2000-579604 B2 20030630 JP 3420751 NO 2001002156 Α 20010702 NO 2001-2156 20010502 PRIORITY APPLN. INFO.: GB 1998-24062 A 19981103 GB 1999-20909 A 19990903 W 19991101 WO 1999-EP8186

OTHER SOURCE(S):

MARPAT 132:321858

GI

Ι

The title compds. [I; R0, R1 = H, halo, alkyl, etc.; R2 = H, alkyl, alkyl AB substituted by one or more fluorine atoms, etc.; R3 = alkyl, NH2] which are potent and selective inhibitors of COX-2 and are of use in the treatment of the pain, fever, inflammation of a variety of conditions and diseases, were prepd. and formulated. E.g., a multi-step synthesis of I [R0 = 3-F; R1 = H; R2 = 6-CF3; R3 = NH2] which showed IC50 of 34 nM against COX-2, was given.

IT 267235-24-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrazolopyridines as selective COX-2 inhibitors)

267235-24-5 HCAPLUS RN

Acetamide, N-[[4-[2-(4-fluorophenyl)-6-(trifluoromethyl)pyrazolo[1,5-CN a]pyridin-3-yl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

8

=> d his

(FILE 'HOME' ENTERED AT 13:45:45 ON 22 JUL 2003)

FILE 'REGISTRY' ENTERED AT 13:45:54 ON 22 JUL 2003

L1 STRUCTURE UPLOADED

L2 8 S L1

186 S L1 FULL L3

FILE 'HCAPLUS' ENTERED AT 13:53:16 ON 22 JUL 2003

9 S L3 L4

L5 3 S L4 AND PD < DECEMBER 1998

L6 2 S L4 AND CAMPBELL, I?/AU

=> s 15 not 16

/ 3 L5 NOT L6 L7

=> d 17, ibib abs fhitstr, 1-3

L7 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Citing References Text

ACCESSION NUMBER: DOCUMENT NUMBER:

1989:95084 HCAPLUS

110:95084

TITLE:

Preparation of new nitrogen-bridged heterocycles. 18. Facile formations of 3-arylpyrazolo[1,5-a]pyridines

and 1-arylindolizines

AUTHOR (S):

Kakehi, Akikazu; Ito, Suketaka; Kinoshita, Naosumi;

Abaka, Yukio

CORPORATE SOURCE:

SOURCE:

Fac. Eng., Shinshu Univ., Nagano, 380, Japan

Bulletin of the Chemical Society of Japan (1988),

61(6), 2055-61

CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE:

LANGUAGE:

OTHER SOURCE(S):

Journal English

CASREACT 110:95084

GI

AB The base treatment of [(benzylthio)methyleneamino]pyridinium I (X = N; R, R1 = H, Me; R2 = Ph, substituted Ph, R3 = SMe, Ph, OEt, NEt2) and [(benzylthio)vinyl]pyridinium bromides I (X = CR4; R, R1 = H, Me; R2 = Ph, substituted Ph, R3 = SMe, R4 = CO2Et, cyano, COPh), possessing an electron-withdrawing substituent such as a nitro or cyano group in the presence or absence of a dehydrogenating agent afforded 3-arylpyrazolo[1,5-a]-pyridines II (X = N) and 1-arylindolizines II (X =CR4) resp. in moderate to good yields, while the reactions of the parent pyridinium salts and those having an electron-releasing group did not produce any significant products. The mode of the reaction, a ring contraction-desulfurization, is the same as that obsd. in related

Π

monocyclic species.

IT 119093-32-2P

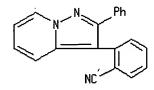
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 119093-32-2 HCAPLUS

Benzonitrile, 2-(2-phenylpyrazolo[1,5-a]pyridin-3-yl)- (9CI) (CA INDEX CN

NAME)



ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2003 ACS on STN

Citing Full References Text

1973:71992 HCAPLUS ACCESSION NUMBER:

78:71992 DOCUMENT NUMBER:

TITLE: Reactive intermediates. XXI. Thermal decarboxylation

of 2,6-diazatricyclo[5.2.1.02,6]deca-4,8-diene-3,10-

diones to pyrazolo[1,5-a]pyridines

AUTHOR (S): Rees, C. W.; Yelland, M.

Chem. Dep., Univ. Leicester, Leicester, UK CORPORATE SOURCE:

Journal of the Chemical Society, Perkin Transactions SOURCE:

1: Organic and Bio-Organic Chemistry (1972-1999)

(**1973**), (3), 221-5

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

Oxidn. of pyrazolin-5-ones (I; R = H, Ph, or CH2Ph) in the presence of AB

tetracyclone gave the corresponding adducts (II), which on heating lost

CO2 and rearranged to the pyrazolo[1,5-a]pyridines (III).

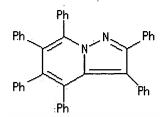
IT 22889-10-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

22889-1<u>0-7</u> HCAPLUS RN

Pyrazolo[1,5-a]pyridine, hexaphenyl- (8CI, 9CI) (CA INDEX NAME) CN



ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2003 ACS on STN

Citing References Text

1969:422062 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 71:22062

TITLE: A novel heterocyclic rearrangement. Extrusion of

carbon dioxide from non-adjacent carbonyl groups

Rees, Charles W.; Yelland, M. AUTHOR (S):

Univ. Leicester, Leicester, UK CORPORATE SOURCE:

SOURCE:

Journal of the Chemical Society [Section] D: Chemical

COMMunications (1969), (8), 377-8 CODEN: CCJDAO; ISSN: 0577-6171

DOCUMENT TYPE:

Journal English

LANGUAGE:

I For diagram(s), see printed CA Issue.

AB Oxidn. of 4-substituted-3-phenyl-2-pyrazolin-5-ones with Pb(OAc)4 in CH2Cl2 contg. tetraphenylcyclopentadienone (I) gave good yields of the Diels-Alder adducts (II). Thermolyses of I at 210°/1 mm. 16 hrs. caused extrusion of CO2 and formation of 30-45% III. The proposed mechanism for this unusual rearrangement involved N-C bond fission (1st part of stepwise retro-Diels-Alder) to give a zwitterion, formation of a lactone produced by attack of the pyrazolone O at the cyclopentenone carbonyl group, and subsequent loss of CO2 with formation of III. The thermolyses also produced 35-40% I, the stable product of the normal retro-Diels-Alder reaction.

IT 22889-10-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 22889-10-7 HCAPLUS

CN Pyrazolo[1,5-a]pyridine, hexaphenyl- (8CI, 9CI) (CA INDEX NAME)

=> file caold

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 27.19 179.95 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -3.26 -3.26

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter <u>HELP FIRST</u> for more information.

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FILE 'REGISTRY' ENTERED AT 13:45:54 ON 22 JUL 2003

STRUCTURE UPLOADED L1

L2/ 8 S L1

186 S L1 FULL L3

FILE 'HCAPLUS' ENTERED AT 13:53:16 ON 22 JUL 2003

9 S L3 L4

L5 3 S L4 AND PD < DECEMBER 1998

L6 2 S L4 AND CAMPBELL, I?/AU

L7 3 S L5 NOT L6

FILE 'CAOLD' ENTERED AT 13:54:45 ON 22 JUL 2003

=> s 13

L80 L3

=> log y

SINCE FILE TOTAL ENTRY SESSION COST IN U.S. DOLLARS

FULL ESTIMATED COST 0.40 180.35

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

0.00 CA SUBSCRIBER PRICE -3.26

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